

Gordon Baym

Statement

and

Readings

Field-Theoretic Methods in Condensed Matter Physics

Gordon Baym

**Department of Physics, University of Illinois at Urbana-Champaign
Urbana, IL, USA**

Abstract

In the late 1950's field-theory techniques began to be introduced into the many-body problem, eventually becoming the common underpinning for the microscopic understanding of condensed matter physics. The major threads in this history were centered in the U.S. and in the Soviet Union. This talk will review the history of these developments, with particular focus on applications of field theory to quantum statistical mechanics and transport theory.

CONSERVATION LAWS AND THE QUANTUM THEORY OF TRANSPORT: THE EARLY DAYS

Gordon Baym

*Department of Physics, University of Illinois at Urbana-Champaign,
1110 W. Green St., Urbana, Illinois 61801, USA*

This talk reviews, from an historical perspective, a chapter in the development of quantum transport theory within the framework of self-consistent non-equilibrium Green's functions.

1 INTRODUCTION

Nearly forty years have sped by since Leo Kadanoff and I worked in Copenhagen on understanding the role of conservation laws and the description of transport in quantum many particle systems. To set the stage for this meeting, I would like to describe here the physics and historical background of our work in these early days.

First a few biographical notes. As the photographs that graced the dust jacket of our 1962 book *Quantum statistical mechanics*¹ show, Leo and I were both in our mid-twenties at the time. When the two of us started life in the 1930's, our parents quite coincidentally lived just about a block apart in Inwood, a neighborhood in upper Manhattan in New York City, mine on Payson Avenue (no. 1 on the map) and his on Seaman Avenue (no. 2). Our immediate neighborhood turned out to be quite a fertile one for theoretical physicists. Roy Glauber grew up in the same apartment building as the Kadanoffs, and Shelly Glashow lived just a block or so away. We all went to the same elementary school (no. 3 on the map), imaginatively named PS52 (PS for "Public School"), and all were at Harvard in the 1950's.

The theorists at Harvard in the late fifties were very excited by recent developments in the many body problem, and particularly by the paper by Paul Martin and Julian Schwinger² on the formalism for finite temperature many body theory³. Even though Leo and I were graduate students in physics at the same time we did not collaborate together until later. Leo worked with Paul Martin, writing a thesis, *Theory of many particle systems: superconductivity*, and with Roy Glauber as well, writing a second thesis, *Acceleration of a particle by a quantized electric field*; I was a student of Julian Schwinger, and wrote only one thesis, *Field theoretic approach to the properties of the solid state*.⁴

Discussing future plans at our graduation in 1960, we found out that we were both independently headed as postdocs in September to Niels Bohr's Institute in Copenhagen – then officially the University Institute for Theoretical

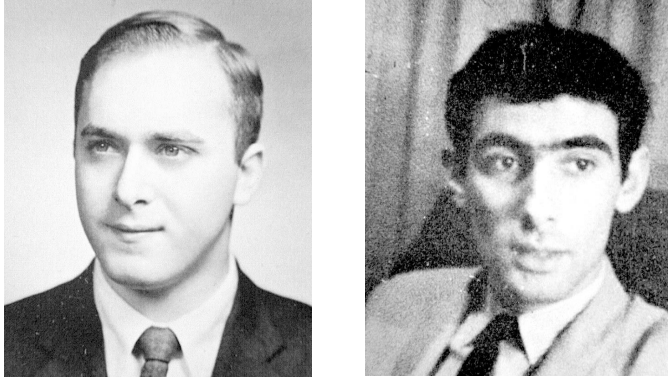


Figure 1: Leo Kadanoff (left) and Gordon Baym (right), circa 1961; from the dust jacket of *Quantum Statistical Mechanics*.

Physics. Copenhagen, with far more bicycles than cars on the streets, was one of the foremost gathering places of physicists from around the world⁵ – a remarkable experience for two fresh Harvard Ph.D.'s. I stayed for two years, and Leo for a little over one year.

2 THE PUZZLES

Since the main emphasis at the Institute at the time was nuclear physics and our focus was on condensed matter problems we had little mentoring from the senior people, with the important exception of Gerry Brown; primarily we worked on our own. Leo's and my collaboration began one day in our first Spring in Copenhagen, when he raised the question of how to construct in the Martin-Schwinger Green's function formalism *approximations* to the two particle propagators that preserved the simple conservation laws. For example, the operator number conservation law,

$$\frac{\partial \rho(rt)}{\partial t} + \nabla \cdot \vec{j}(rt) = 0, \quad (1)$$

implies that correlation functions of the density and current with an arbitrary operator, $\mathcal{O}(r't')$, should obey

$$\begin{aligned} \frac{\partial}{\partial t} \langle T(\rho(rt)\mathcal{O}(r't')) \rangle + \nabla \cdot \langle T(\vec{j}(rt)\mathcal{O}(r't')) \rangle \\ = \langle [\rho(rt), \mathcal{O}(r't)] \rangle \delta(t - t'). \end{aligned} \quad (2)$$

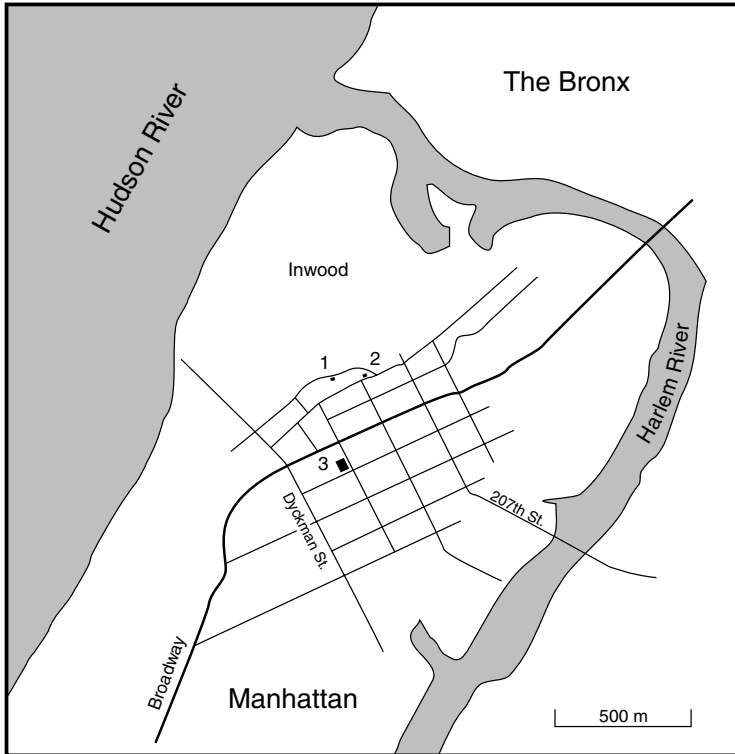


Figure 2: The Inwood area of upper Manhattan.

where T denotes time-ordering of the operators.

Leo's interest in the problem arose from the question of how to write the BCS theory of superconductivity in a way that would yield correctly the Anderson mode – the longitudinal collective oscillation of a neutral superconductor^b (now famous in high energy physics as the Higgs boson). As originally formulated the BCS theory did not give two-particle correlation functions that obeyed the number conservation condition (2). Equivalently, the problem was how to build local gauge invariance into the theory. The more general issue was how to construct, within the Green's function formalism, consistent quantum theories of transport. This problem was nagging me too, because, as Paul Martin pointed out at my doctoral defense, I had essentially gotten it wrong in my thesis. In trying to calculate sound wave damping in a metal via simple

Green's function approximations, I was missing a factor of 4/5 compared with a calculation via the Boltzmann equation. Paul immediately realized that the lack of this factor indicated a conceptual error in the underlying physics. It is very hard to get a factor of five from simple mistakes – in this case it comes from $\int P_2(\cos \theta)^2$, which arises from correctly including the scattering back-into-the-beam term in the transport equation. Leo's and my problems were closely related.

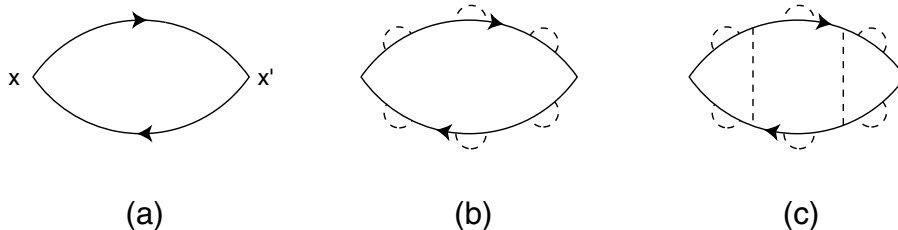


Figure 3: (a) The one loop approximation, (b) the self-energy corrections on the lines that are included, and (c) scattering into-the-beam corrections.

To see how approximations can fail obey to the conservation laws consider going beyond the lowest order evaluation of the density-density and current-density correlation functions in the Hartree-Fock approximation, i.e., as a single loop of Green's functions. The lowest order calculation, Fig. 3a, in which the lines are Hartree-Fock Green's functions, obeys the conservation laws. The trouble starts when one tries to improve the Green's functions beyond lowest order, including better self-energies, as shown in Fig. 3b, but not vertex corrections. In the one loop approximation, the density-density correlation function, in imaginary time, is given (in the notation of Ref. 1) by

$$\langle T(\rho(rt)\rho(r't')) \rangle = \mp T^2 \sum_{\nu\nu'} \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} G(p, z_\nu) G(p', z_{\nu'}) \times e^{i(\vec{p}-\vec{p}')\cdot(\vec{r}-\vec{r}')} e^{-i(z_\nu-z_{\nu'})(t-t')}. \quad (3)$$

The current-density correlation function is similarly

$$\langle T(\vec{j}(rt)\rho(r't')) \rangle = \mp T^2 \sum_{\nu\nu'} \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} \frac{\vec{p}+\vec{p}'}{2m} G(p, z_\nu) G(p', z_{\nu'}) \times e^{i(\vec{p}-\vec{p}')\cdot(\vec{r}-\vec{r}')} e^{-i(z_\nu-z_{\nu'})(t-t')}. \quad (4)$$

Trying to see if the correlation functions obey the number conservation law,

Eq. (1), we find, using Dyson's equation for the Green's functions,

$$G^{-1}(p, z) = z - \frac{p^2}{2m} + \Sigma(p, z), \quad (5)$$

that

$$\begin{aligned} & \frac{\partial}{\partial t} \langle T(\rho(rt)\rho(r't')) \rangle + \nabla \cdot \langle T(\vec{j}(rt)\rho(r't')) \rangle \\ &= \pm iT^2 \sum_{\nu\nu'} \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} (\Sigma(p, z_\nu) - \Sigma(p', z_{\nu'})) G(p, z_\nu) G(p', z_{\nu'}) \\ & \quad \times e^{i(\vec{p}-\vec{p}') \cdot (\vec{r}-\vec{r}')} e^{-i(z_\nu - z_{\nu'})(t-t')}. \end{aligned} \quad (6)$$

The right side, which involves the difference of the self-energies, does not vanish in general beyond the Hartree-Fock approximation. Even with a constant particle lifetime, τ , corresponding to scattering by random impurities, the correlation functions fail to obey the conservation laws. For a constant lifetime the spectral function of G is

$$A(p, \omega) = \frac{1/\tau}{(\omega - p^2/2m)^2 + 1/4\tau^2}, \quad (7)$$

with the corresponding self-energy given by $\Sigma(z) = \pm i/2\tau$ (where the + sign is for the complex frequency z in the upper half plane, and the - sign for z in the lower half plane). In order to include the conservation laws correctly it is necessary to include the scatterings between the two lines, as shown in Fig. 3c; these correspond to including the scattering back-into-the-beam terms in the Boltzmann equation.

The subtle feature of the problem of the correlation functions obeying the conservation laws was that it was not sufficient merely to include particle number and momentum conservation at the individual vertices in a diagrammatic expansion. Simple approximations to the correlation functions need not obey the conservation laws, even though particle number and momentum are conserved at the individual vertices.

The second piece of the puzzle of constructing a quantum theory of transport phenomena was that it required summation of an infinite set of diagrams. Let me illustrate the point by means of the simple example of the electrical conductivity of a metal. Consider first the trivial example of classical carriers of charge e moving at velocity \vec{v} in the presence of an electrical field $\vec{E}(t)$ and a friction force described by a scattering time τ . Newton's equation reads

$$m \frac{d\vec{v}}{dt} = e\vec{E}(t) - m \frac{\vec{v}}{\tau}; \quad (8)$$

for an electric field of frequency ω , the velocity is,

$$\vec{v}(\omega) = \frac{e}{m} \frac{\vec{E}(\omega)}{-i\omega + 1/\tau}. \quad (9)$$

Since the electrical current produced is $\vec{j} = ne\vec{v} = \sigma\vec{E}$, one finds the complex conductivity,

$$\sigma(\omega) = \frac{ne^2}{m} \frac{\tau}{1 - i\omega\tau}, \quad (10)$$

whose real part,

$$\text{Re}(\sigma) = \frac{ne^2}{m} \frac{\tau}{1 + \omega^2\tau^2}, \quad (11)$$

determines the dissipation. In the collisionless regime, $\omega\tau \gg 1$, $\text{Re}(\sigma) \propto \tau^{-1}$, i.e., proportional to the scattering rate, or scattering matrix elements, $M_{\vec{p}\vec{p}'}$, squared. This result follows directly from perturbation theory. On the other hand, in the collision-dominated regime, $\omega\tau \ll 1$, the dissipation $\text{Re}(\sigma) \propto \tau$, is *inversely* proportional to the matrix elements squared, a very difficult result to derive by summing diagrams in perturbation theory.

The standard derivation of the conductivity in terms of scattering matrix elements is via the Boltzmann equation, which for electrons scattering on impurities reads,

$$\begin{aligned} \frac{\partial f_{\vec{p}}}{\partial t} + \vec{v}_{\vec{p}} \cdot \nabla_{\vec{p}} f_{\vec{p}} - e\vec{E} \cdot \nabla_{\vec{p}} f_{\vec{p}} \\ = - \int \frac{d^3p'}{(2\pi)^3} 2\pi |M_{\vec{p}\vec{p}'}|^2 \delta(\epsilon_{\vec{p}} - \epsilon_{\vec{p}'}) [f_{\vec{p}}(1 - f_{\vec{p}'}) - f_{\vec{p}'}(1 - f_{\vec{p}})]. \end{aligned} \quad (12)$$

Linearizing the distribution function in the form $f_{\vec{p}} = f_{\vec{p}}^0 + \nabla_{\vec{p}} f_{\vec{p}}^0 \cdot \vec{u}$, one readily finds from Eq. (12) that

$$\vec{u} = e\vec{E} \frac{\tau_{\text{tr}}}{1 - \omega\tau_{\text{tr}}}, \quad (13)$$

and

$$\sigma = \frac{ne^2}{m} \frac{\tau_{\text{tr}}}{1 - i\omega\tau_{\text{tr}}}, \quad (14)$$

as in Eq. (10). Here the transport scattering time is given by

$$\frac{1}{\tau_{\text{tr}}} = - \int \frac{d^3p'}{(2\pi)^3} 2\pi |M_{\vec{p}\vec{p}'}|^2 \delta(\epsilon_{\vec{p}} - \epsilon_{\vec{p}'}) (1 - \cos\theta_{\vec{p}\vec{p}'}). \quad (15)$$

The $\cos\theta\vec{p}\vec{p}'$ term is a result of the scattering back into the beam, described by the final $f_{\vec{p}'}(1 - f_{\vec{p}})$ collision term on right side of Eq. (12).

The conductivity is given more generally in terms of the current-current correlation function, $\langle jj \rangle(z)$ (e.g., the Fourier transform of the retarded commutator) by

$$\sigma(\omega) = \frac{i}{\omega} \left(\langle jj \rangle(\omega + i\eta) + \frac{n}{m} \right). \quad (16)$$

To derive the low frequency limit from a diagrammatic expansion of the correlation function in terms of Green's functions, one must sum an infinite set of diagrams, and to find the correct transport coefficients, include the scattering back-into-the-beam terms corresponding to Fig. 3c. The Boltzmann equation carries out such a summation brilliantly. The failure of approximate correlation functions to include the conservation laws meant that one could not correctly describe low frequency long wavelength transport phenomena, so well accounted for by the Boltzmann equation. The challenges facing us in building theories of quantum transport were thus to learn how to include the conservation laws in approximations to the correlation functions, and how, from Green's functions, to recover and generalize the basic structure of the Boltzmann equation.

3 SELF-CONSISTENT APPROXIMATIONS

Furiously scribbling all evening after Leo posed his question, I began to see how to include the conservation laws in two point correlations functions in terms of self-consistent approximations. The starting point was to include in imaginary time, from 0 to $-i\beta$, an external potential coupled, e.g., to the density:

$$H_{\text{ext}}(t) = \int d^3r \rho(rt) U(rt). \quad (17)$$

The single particle Green's function then takes the form,

$$G(12; U) = -i \frac{\text{tr} \left[e^{-\beta(H - \mu N)} T \left(e^{-i \int dt H_{\text{ext}}} \psi(1) \psi^\dagger(2) \right) \right]}{\text{tr} \left[e^{-\beta(H - \mu N)} T \left(e^{-i \int dt H_{\text{ext}}} \right) \right]} \quad (18)$$

where T defines the time ordering along the imaginary time path, and the time integrals are from 0 to $-i\beta$. The next step was to choose an approximation for the two particle Green's function $G_2(U)$ in $[0, -i\beta]$, e.g., the Hartree-Fock approximation illustrated in Fig. 4a. From this G_2 we constructed the single

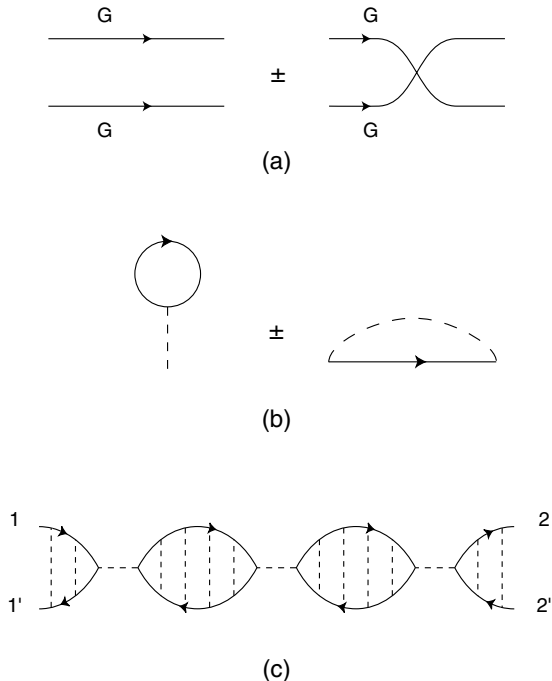


Figure 4: The procedure for deriving conserving approximations for the two particle correlation functions. Illustrated here for the Hartree-Fock approximation, in (a) one chooses an initial approximation to the two particle Green's function, in (b) constructs the single particle self-energy from it, and in (c) constructs the conserving two particle correlation function by differentiating the self-consistent one particle Green's function.

particle self-energy Σ , as shown in Fig. 4b in Hartree-Fock. The single particle Green's function, $G(U)$, obeys Dyson's equation (5) self-consistently. The key step now was to generate the two particle correlation function as a variational derivative of $G(U)$, via

$$\frac{\delta G(1, 1'; U)}{\delta U(2)} \Big|_{U=0} = \pm [G_2(12, 1'2^+) - G(11')G(22^+)] \Big|_{U=0} \equiv \pm L(12, 1'2^+). \quad (19)$$

Figure 4c shows the resulting correlation function generated from the initial Hartree-Fock approximation, the random phase approximation with a sum of particle-hole ladders across the bubbles. For any starting approximation to G_2 , the two particle correlation function generated as a variational derivative

obeys the differential conservation laws.⁷

Leo and I immediately wrote up our first and only journal paper together, *Conservation laws and correlation functions*.⁸ In preparing for this talk, I scoured through old notes in Urbana, and came upon the original typewritten draft of the paper, which contains both Leo's and my handwriting, titled, *Conservation laws and the quantum theory of transport*. Recognizing his pivotal role in the development we listed Paul Martin as a prospective author, but he modestly declined to be on the masthead. His name is crossed out in the draft, and he is finally acknowledged for discussions that established the form of the conservation laws obeyed by the two particle correlation functions. We recognize in the draft that the self-consistent approximations for the two particle correlation functions yield linearized Boltzmann equations. After discussing the self-consistent T -matrix approximation for the self-energy of the single particle Green's function G , we note that, "In the long wavelength limit the L equation leads to a generalization of the linearized Boltzmann equation in which the scattering cross section is proportional to $|T|^2$. This generalization reduces in turn to an ordinary Boltzmann equation in the low density limit. Thus our procedure enables us to derive the linearized Boltzmann equation from an equation which defines $G(U)$ from a sum of ladder diagrams." Similarly, we mention deriving a Boltzmann equation from the shielded potential approximation, and finally, we promise that "the derivation of the generalized Boltzmann equations will be given in future publications." The published paper strangely contains no mention of the Boltzmann equation. We did return, however, to Boltzmann equations in our book.

At Gerry Brown's instigation, we gave a series of lectures on the quantum many body problem in Copenhagen, and then to Ivar Waller's group in Uppsala in the Spring of 1961, and in following Fall to Wiesław Czyż's group in Krakow and at the Institute for Nuclear Studies at Hoża 69 in Warsaw. These lectures became the basis for our book. Writing the book was great fun; either we would sit together and write from scratch – actually Leo paced up and down non-stop, while I sat putting pen to paper – or often Leo would come in, in the morning, with the draft of a new chapter, which we would then revise. The whole book-writing took, it seemed, less than a month. I recall the conversation with Leo about the order of authors names on the book. Since on our first paper, my name, being earlier in the alphabet than his, came first, he suggested that it would be fair if we alternated our names on subsequent publications; thus the book became Kadanoff-Baym.

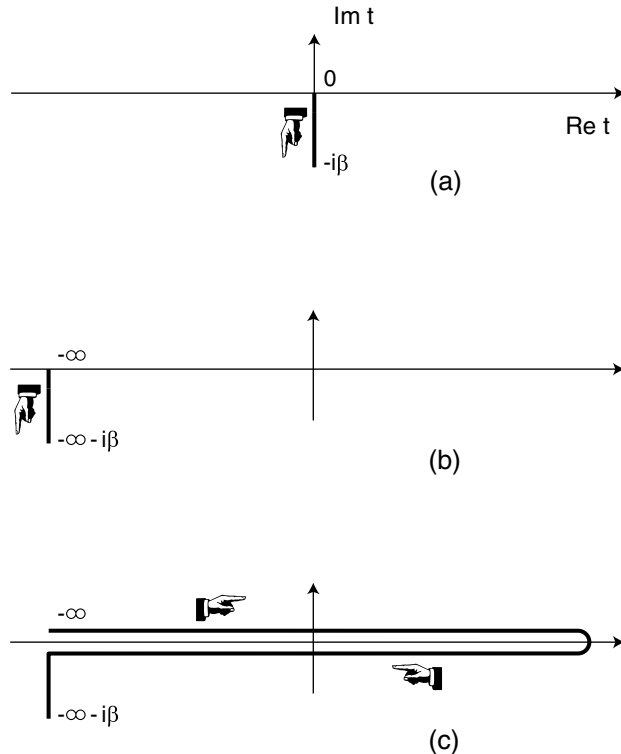


Figure 5: The succession of contours in deriving generalized Boltzmann equations, from (a) the usual contour in imaginary time, shifted to $-\infty$ in (b), and distorted to (c), the real time round-trip.

3.1 Generalized Boltzmann equations

A good part of the book is devoted to deriving generalized Boltzmann equations from self-consistent approximations for the Green's functions, a procedure for which Leo deserves full credit. The method begins with the Green's function in the presence of an external potential, Eq. (18) on $[0, -i\beta]$, Fig. 5a, as we studied in Ref. 7. The contour of integration is then shifted back to $[-\infty, -\infty - i\beta]$, as shown in Fig. 5b, and then distorted to the "round-trip" contour from $-\infty$ to $+\infty$ and back again to $-\infty$ to $-\infty - i\beta$. The Green's function is given on

the round-trip contour by,

$$G(12; U) = -i \frac{\text{tr} \left[e^{-\beta(H-\mu N)} T \left(e^{-i \oint dt H_{\text{ext}}} \psi(1) \psi^\dagger(2) \right) \right]}{\text{tr} \left[e^{-\beta(H-\mu N)} T \left(e^{-i \oint dt H_{\text{ext}}} \right) \right]} \quad (20)$$

where now T defines the time ordering along the round-trip path, as shown in Fig. 5c, imaginary time path, and the time integrals are along the path. The external potential need not be the same on the two sectors of the contour along the real axis. The Green's function on the path obeys,

$$\left(i \frac{\partial}{\partial t} + \frac{\nabla^2}{2m} - U(rt) \right) G(rt, r't') - \oint \Sigma(rt, \bar{r}\bar{t}) G(\bar{r}\bar{t}, r't') = \delta(r - r') \delta(t - t'). \quad (21)$$

To derive the generalized non-linear Boltzmann equation, we write the distribution function in the Wigner form,

$$g^<(p\omega RT) = \int dr dt e^{-ip \cdot r + i\omega t} \langle \psi^\dagger(1') \psi(1) \rangle \quad (22)$$

where $r = r_1 - r'_1$, $t = t_1 - t'_1$ and $R = (r_1 + r'_1)/2$, $T = (t_1 + t'_1)/2$. A new feature here was to treat the energy of the particles, ω , as a variable independent of their momentum p , thus allowing one to go beyond situations with well-defined quasiparticles. Expansion of the single particle Green's function equations on the path for disturbances slowly varying in both space and time, yields the generalized Boltzmann equation, on which we are focussing at this meeting,

$$\begin{aligned} \frac{\partial g^<}{\partial t} + \frac{\partial g^<}{\partial \omega} (U + Re\Sigma) + \frac{p}{m} \cdot \nabla_R g^< - \nabla_R (U + Re\Sigma) \cdot \nabla_p g^< \\ + \frac{\partial Re g}{\partial \omega} \frac{\partial \Sigma^<}{\partial t} - \frac{\partial Re g}{\partial t} \frac{\partial \Sigma^<}{\partial \omega} + \nabla_p Re g \cdot \nabla_R \Sigma^< - \nabla_R Re g \cdot \nabla_p \Sigma^< \\ = -\Sigma^> g^< + \Sigma^> g^<. \end{aligned} \quad (23)$$

Here

$$\begin{aligned} g(pzRT) &= \int \frac{d\omega}{2\pi} \frac{(g^> + g^<)(p\omega RT)}{z - \omega} \\ &= \frac{1}{z - p^2/2m - U(RT) - \Sigma(pzRT)}. \end{aligned} \quad (24)$$

Understanding how to derive general Boltzmann equations from the many body formalism put the development of quantum transport theory on a firm

foundation. As we wrote, “Our rather elaborate Green’s function arguments . . . provide a means of describing transport phenomena in a self-contained way, starting from a dynamical approximation, i.e., an approximation for $G_2(U)$ in terms of $G(U)$. These calculations require no extra assumptions. The existence of local thermodynamic equilibrium is derived from the Green’s function approximations. The various quantities that appear in the conservation laws are determined by the approximation. The theory provides at the same time a description of what transport processes occur . . . and a determination of the numerical quantities that appear in the transport equations.”⁹ Finally, we could derive the sound velocity of a gas from the Schrödinger equation.

3.2 Round-trip Green’s functions

A crucial ingredient in the derivation of Boltzmann equations was the use of Green’s functions defined on the round-trip contour along the real axis. The method was invented by Schwinger, and presented in his lectures on Brownian motion at the Brandeis summer school in 1960, where I became familiar with it. Although the lectures were unpublished, Schwinger did write up the ideas in his paper *Brownian motion of a quantum oscillator*.¹⁰ As was always characteristic of Schwinger, not a diagram appears in the paper. Feynman put it well in his *Talk at the First Schwinger Festspiel* at the banquet for Schwinger on his sixtieth birthday in 1978, reminiscing about their conversation at the 1948 Pocono conference: “He [Schwinger] would say, well I got a creation and then another annihilation of the same photon and then the potential goes . . . I’d draw a picture that looks like this. He didn’t understand my pictures and I didn’t understand his operators, but the terms corresponded and by looking at the equations we could tell . . . that we had both come to the same mountain”¹¹

The round-trip technique was also employed in the context of quantum electrodynamics in 1961-62 by Kalyana T. Mahanthappa, a fellow Schwinger graduate student at Harvard, and Pradip Bakshi, a slightly later student of Schwinger’s.^{12,13} Actually, Robert Mills (of Yang-Mills), while at the University of Birmingham in 1962, wrote but did not publish, a lovely set of notes on round-trip Green’s function techniques,¹⁴ which formed the basis for his later book.¹⁵ He refers in these notes to Schwinger’s 1961 paper, and remarks that, “The present work, some of which has, I believe, been duplicated independently by Baym and Kadanoff, following the methods of Martin and Schwinger, makes use of the thermodynamic Wick’s theorem of Matsubara and Thouless, and others, with the integration contour in the complex time plane distorted to include the real axis.” The method was then used by Leonid Keldysh in the

Soviet Union, described first in his 1964 paper.¹⁶ Our book was translated into Russian in the same year¹⁷ but Keldysh did not refer to it, writing rather, “Our diagram technique will be close to Mills’ technique for equilibrium systems,” citing Mills’ notes. Schwinger influence was widely felt.

$$\Phi = \frac{1}{2} \begin{array}{c} \circlearrowleft \\ | \\ \circlearrowright \end{array} \pm \frac{1}{2} \begin{array}{c} \circlearrowleft \\ \text{---} \\ \circlearrowright \end{array} \Rightarrow \Sigma = \begin{array}{c} \circlearrowleft \\ | \\ \text{---} \end{array} \pm \begin{array}{c} \text{---} \\ \text{---} \end{array}$$

(a)

$$\Phi = \sum_n \frac{1}{n} \begin{array}{c} \circlearrowleft \\ \text{---} \\ \circlearrowright \end{array} \Rightarrow \Sigma = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array}$$

(b)

$$\Phi = \sum_n \frac{1}{n} \begin{array}{c} \circlearrowleft \\ \text{---} \\ \circlearrowright \end{array} \Rightarrow \Sigma = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array}$$

(c)

Figure 6: Φ and the corresponding self-energies Σ for (a) the self-consistent Hartree-Fock approximation, (b) the self-consistent T-matrix approximation, (c) the shielded potential approximation.

3.3 Φ -derivable approximations

Leo left Copenhagen in late 1961 to accept an Assistant Professorship at the University of Illinois in Urbana, then one of the few centers of activity in many body physics. I was offered the same irresistible position at Illinois shortly after Leo arrived, but stayed in Copenhagen until September 1962 and then spent a year at Berkeley before going to the midwest. The problem that intrigued me in Copenhagen was how to delineate the structure of approximations to multiparticle Green’s functions that would include the conservation laws.¹⁸ The key turned out to be to start with a functional $\Phi[G]$ of the fully self-consistent Green’s function, G , from which one generates the self-energy self-consistently

as a variational derivative of Φ with respect to G :

$$\delta\Phi[G] = \text{tr} \Sigma \delta G. \quad (25)$$

The Green's function, G , then self-consistently obeys Dyson's equation with the self-energy, Σ , given by Eq. (25). The procedure is illustrated in Fig. 6, which shows Φ and the corresponding self-energies for the self-consistent Hartree-Fock, T-matrix, and shielded potential approximations. All correlations derived as variational derivatives then obey the conservation laws. The method made clear the relations between the conservation laws at the vertices and the macroscopic conservation laws. An extra bonus of this procedure was that various methods of calculating the thermodynamics from the self-consistent G , e.g., coupling constant integration, all lead to the same result for the partition function,¹⁹

$$\ln Z = \pm[\Phi[G] - \text{tr} \Sigma G + \text{tr} \log(-G)]. \quad (26)$$

In the early 1960's we could only apply the transport theory to a limited number of essentially exactly soluble problems, e.g., systems near local thermodynamic equilibrium, and the Landau theory of the normal Fermi liquid. The present explosion in computing power now offers the possibility of solving self-consistent approximations numerically, as in the GW method in solids based on the shielded-potential approximation.^{20,21} Extensions of the approach to systems with condensates,²²⁻²⁴ and to relativistic systems, including electrodynamic and quark-gluon plasmas, both in equilibrium and non-equilibrium,²⁵⁻²⁷ open new windows to deal with systems of current experimental interest such as Bose condensed atomic clouds and ultrarelativistic heavy-ion collisions. As we see from the entirety of papers at this conference, we are standing on the threshold of a much deeper understanding of transport and equilibrium phenomena in a wide variety of interacting systems.

Acknowledgements

I would first like to express my gratitude to Michael Bonitz for organizing this meeting. His extraordinary efforts have given us a wonderful opportunity to learn about the recent progress made in harvesting the fruits of the little seedlings planted many years ago. I would also like to thank Michael Baym for preparing the graphics. It is a pleasure to acknowledge support by the U.S. National Science Foundation, from my early years in Copenhagen as a National Science Foundation Postdoctoral Fellow, through to current Grant No. PHY98-00978.

References

1. L.P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W.A. Benjamin, New York, 1962).
2. P.C. Martin and J. Schwinger, *Phys. Rev.* **115**, 1342 (1959).
3. Paul Martin, in his accompanying talk at this meeting, paints a vivid picture of the theoretical physics milieu at Harvard revolving around Schwinger in this era.
4. G. Baym, Harvard University (1960), unpublished. *Annals of Phys.* (N.Y.) **14**, 1 (1961).
5. A charming history of the beginning of Niels Bohr's Institute is P. Robinson, *The Early Years; the Niels Bohr Institute 1921-1930* (Akademisk Forlag, Copenhagen, 1979).
6. P.W. Anderson, *Phys. Rev.* **112**, 1900 (1958).
7. The variational derivative technique, which turned into a powerful tool in the many body problem, was originated by Schwinger in his papers on quantum field theory in *Proc. Nat. Acad. Sci.* **37**, 379, 382 (1951). See Paul Martin's talk in this volume for further discussion of these remarkable papers. I learned how to apply the technique from the unpublished *Lecture notes on quantum field theory* (Naval Research Laboratory, 1955) by Richard Arnowitt, an earlier student of Schwinger's.
8. G. Baym and L.P. Kadanoff, *Phys. Rev.* **124**, 287 (1961).
9. Ref. 1, p. 138.
10. J. Schwinger, *J. Math. Phys.* **2**, 407 (1961).
11. R. P. Feynman, *Themes in Contemporary Physics II, Essays in honor of Julian Schwinger's 70th birthday*, S. Deser and R. J. Finkelstein, eds. (World Scientific, Singapore, 1989) pp. 92-93.
12. K. T. Mahanthappa, *Phys. Rev.* **126**, 329 (1962).
13. P. M. Bakshi and K. T. Mahanthappa, *J. Math. Phys.* **4**, 1, 12 (1963).
14. R. Mills, *Propagators for quantum statistical physics*, unpublished, 1962.
15. R. Mills, *Propagators for many-particle systems*, 1969.
16. L. Keldysh, *Zh. Eksp. Teor. Fiz.* **47**, 1515 (1964) [Engl. transl., *Sov. Phys. JETP* **20**, 1018 (1965)].
17. L.P. Kadanoff and G. Baym, *Kvantovaya Statisticheskaya Mehanika* (Izdatelstvo "Mir," Moscow, 1964). The Russian edition was published at the munificent price of 77 kopecks. In late 1964 Leo brought back to Urbana the 500 rubles in royalties we were given for the translation – in the form of caviar; the ensuing party was quite memorable.
18. G. Baym, *Phys. Rev.* **127**, 1391 (1962).
19. This relation between the partition function and the functional Φ was

- first derived for the exact theory by J. M. Luttinger and J. C. Ward, *Phys. Rev.* **118**:1417 (1960).
20. Reviewed in W.G. Aulbur, L. Jönsson, and J.W. Wilkins, *Solid State Phys.* **54**, 1 (1999).
 21. C.-O. Almbladh, talk at this meeting; C.-O. Almbladh, U. von Barth, and R. van Leeuwen, *J. Mod. Phys. B*, vol. 13, p. 535 (1999).
 22. W. Götze and H. Wagner, *Physica* **31**, 475 (1965).
 23. G. Baym and G. Grinstein, *Phys. Rev.* **D15**:2897 (1977).
 24. A. Griffin, *Phys. Rev.* **B53**, 9341 (1996); M. Imamović-Tomasović and A. Griffin, this volume.
 25. B. Vanderheyden and G. Baym, *J. Stat. Phys.* **93**, 843 (1998); and this volume.
 26. Y. B. Ivanov, J. Knoll, and D. N. Voskresensky, this volume.
 27. J.-P. Blaizot and E. Iancu, *Nucl. Phys.* **B557**, 183 (1999).

Out of the Crystal Maze

Chapters from the History of Solid-State Physics

Edited by

LILLIAN HODDESON

University of Illinois

ERNEST BRAUN

Open University

JÜRGEN TEICHMANN

Deutsches Museum

SPENCER WEART

American Institute of Physics

New York Oxford

OXFORD UNIVERSITY PRESS

1992

The highly mathematical renormalization group techniques later developed by Leo Kadanoff, Ben Widom, Kenneth Wilson, and others would eventually provide new physical insights into the partition function and correlation functions near critical points, and into the nature of critical scattering.⁵¹⁸

In the 1950s the technology of high- and low-temperature series expansions continued to be developed, particularly in England, and was applied to the Heisenberg as well as the Ising model.⁵¹⁹ At low temperatures, the series expansion technique resembled the earlier spin-wave approximations for the Heisenberg model. The expansions of Domb, Rushbrooke, and co-workers were distinguished from other approximation methods in that the procedure was systematic and based on exact power series expansions of the free energy. Although at first sight the series expansions were a numerical method offering no physical insight, the combinatorial problem in calculating coefficients in the series did entail physical considerations suggestive of the processes entailed in critical behavior. The series expansions permitted estimation with considerable accuracy of the behavior of thermodynamic functions close to the critical point. Furthermore, they applied to three as well as two dimensions, and to the Heisenberg and other models as well as to the Ising case. Beginning in 1961, the technology would be supplemented by bringing to bear the tool of Padé approximants, which provided a means for continuing the series results to the critical point.

One of the most important developments in statistical mechanics in the postwar period was the introduction of field-theory techniques, modeled initially on quantum electrodynamics. We have earlier traced their development in the context of the electron gas and have noted their use in the problems of superconductivity and liquid helium. Eventually, the field theory approach would become a common underpinning for nearly all the various areas of the many-body problem. By 1961, Pines could appropriately say that “the recent developments in the many-body problem . . . have tended to change it from a quiet corner of theoretical physics to a major crossroad.”⁵²⁰

The application of field theory to statistical mechanics had analogies with earlier cluster expansions and with the use of coupled integral equations for classical n -particle distribution functions. In the 1940s the classical coupled integral equations for the distribution functions had been developed by Born and Green, Kirkwood, and Bogoliubov.⁵²¹

The use of diagrams in the finite temperature quantum many-body problem may be traced in large measure to the pioneering work of Takeo Matsubara at the Research Institute for Fundamental Physics in Kyoto in 1955.⁵²² Matsubara approached the calculation of the partition function of many-body systems with interactions by introducing “explicitly the quantized field of particles and utiliz[ing] the various techniques of operator calculus in quantum field theory as far as possible in evaluating the quantum-statistical average of the field quantities.” As he stated in his abstract,

the grand partition function, which is a trace of the density matrix expressed in terms of field operators, can be evaluated in a way almost parallel with the evaluation of the vacuum expectation values of the S -matrix in quantum field theory, provided that appropriate modifications in notation and definition are made.

Some physicists developed perturbation theories for the many-body problem at finite temperatures, and time-dependent Green's functions (generalization of those introduced by Matsubara) were variously defined, the differential equations they satisfy derived, and theorems about them proved. Crucial to making thermal Green's functions into a practical calculational tool was the discovery by Ryogo Kubo of the boundary conditions that they obey. The boundary conditions, a form of periodicity in imaginary time, exploited the similarity, first recognized by Felix Bloch in his 1932 *Habilitationschrift* (Chapter 2), of the thermal density matrix and the Heisenberg time-development operator for imaginary times.⁵²³ Primarily, interest lay in understanding normal properties of metals, superconductivity, and superfluidity. Field-theory methods and language were eventually brought to bear on critical phenomena, and by the early 1970s, Wilson could rightly state that "the efforts of many years to apply Feynman diagram methods to critical phenomena finally succeeded."⁵²⁴

How far had physicists come by the 1960s in understanding phase transitions? The question concerns underlying scientific objectives—how different researchers would define an "adequate understanding" of phase transitions and critical phenomena. Ernst Mach might have considered it sufficient for an elaborate numerical calculation based on the canonical ensemble to yield the experimental curves for thermodynamic functions in the critical region. Ehrenfest might have insisted rather that physical insight into the nature of the process is of central importance. Philosophical attitudes, rarely articulated in the published articles, were muted by the positivism dominating physics in the United States and Western Europe since the Second World War. The inclinations of leading physicists of an earlier generation—Bohr, Einstein, Planck, Schrödinger—had been intensely philosophical; Bloch and Peierls, by contrast, expressed a sentiment characteristic of the younger generation when they complained of Bohr's preoccupation with fundamental issues as a distraction from the challenging task of physics to calculate answers.⁵²⁵ By the end of the Second World War, the antiphilosophical bias had hardened among physicists.⁵²⁶

The appeal of a theory of phase transitions was that it could potentially encompass the most diverse physical systems. To the extent that the primary objective of such a theory was to provide a simple and lucid description of the physical and mathematical origin and nature of the discontinuities and singularities of otherwise smooth functions describing macroscopic matter, the Weiss field and early kinetic theory models, such as that of van der Waals, had been major steps. But adequate mathematical description required exact calculations so complex as to constitute a subject of study in their own right; the primary objective might appear, at least temporarily, forgotten. Increasingly after the war the focus was on the exact nature of the singularities and the precise "critical exponents."

The discrepancy between the logarithmic singularity of the Onsager solution and all previous results had highlighted the issue. Once identified as crucial, the question could and did engender a variety of approaches and a fairly well-defined general research program to calculate and measure those exponents. The laborious series expansions were a natural and fruitful part of such a research program. The thermodynamic theories reflected the natural requirement that phase transitions and critical phenomena had somehow to fit into general thermodynamics, and the

description in terms of correlation functions, so closely related to scattering experiments, fluctuations, and the theory of steady-state irreversible phenomena, linked critical phenomena to other portions of physics. Through subsequent progress by renormalization group techniques, coupled with extensive computer simulation, the theory of critical phenomena came to fruition.

8.3 Conclusion

A number of common themes and elements unify the subfields of collective phenomena. Among them are the concepts of long-range order, changes of symmetry in phase transitions, collective modes, low-lying excitations above the ground state, Bose–Einstein condensation, pairing, broken symmetry, order parameters, and macroscopic quantum phenomena. Although certain of these unities were recognized well before the Second World War, even though often phrased in different language, recognition alone did not weld the subfields together. And although individuals did occasionally cross over among subfields in their work (e.g., Landau on helium, superconductivity, and phase transitions; Fritz London on superconductivity and helium), the communities of researchers working on different problems of collective phenomena did not generally see themselves as working under a common umbrella. Only very gradually, in the 1950s and 1960s, did these subcommunities and subfields coalesce around the unifying strands.

As an illustration of the intellectual unification of the subfields, consider the development of the concept of a spatially varying order parameter to describe the broken-symmetry states of superconductivity and superfluidity. The notion of an order parameter distinguishing a condensed state can be traced back to the local magnetization in the Weiss theory of ferromagnetism (Chapters 2 and 6). Bloch, in his *Habilitationsschrift* on ferromagnetic domain walls, then generalized the notion to spatially varying situations and showed how to calculate the energy in terms of the order parameter.⁵²⁸ The idea was soon picked up by Landau in his 1935 theory of phase transitions,⁵²⁹ and was eventually introduced into superconductivity in the 1950 Ginzburg–Landau theory.⁵³⁰ With Gor'kov's 1957 formulation of the BCS theory of superconductivity in terms of diagrammatic field theory and his subsequent derivation of the Ginzburg–Landau theory from BCS, the role of a spatially varying order parameter characterizing the superconducting state became established.⁵³¹

The recognition of an order parameter to describe superfluidity in helium came through a basically independent route. The idea was implicit in London's 1938 picture of helium undergoing Bose–Einstein condensation into a single macroscopic quantum state,⁵³² and was also probably in the back of Onsager's mind when he argued, in 1949, that the vorticity had to be quantized. (He certainly understood its role in superconductivity by the time of the flux quantization experiments.) As early as 1951, O. Penrose suggested how the single-particle correlation function of a Bose fluid would exhibit long-range order in terms of what we now recognize as the order parameter.⁵³³ But an order parameter that was possibly spatially varying did not enter into any discussion of the microscopic behavior of helium II until the work of Pitaevskii and Gross in 1961.⁵³⁴ Aside from quantization of circulation, the

concept would become useful only when Josephson and Anderson, in the context of tunneling between superconductors, demonstrated the importance of the phase of the order parameter.⁵³⁵ The commonality of the order parameters used to describe the broken symmetry in both superconductivity and helium superfluidity was recognized by workers in the field by the early 1960s, and was codified in Yang's review of "off-diagonal" long-range order.⁵³⁶ By this point, the two phenomena were seen as similar manifestations of quantum mechanics on a macroscopic scale.

The growing application in the late 1950s of diagrammatic field-theory methods (Feynman diagrams and Green's functions) led to a general theoretical framework for collective phenomena. Although the first diagrammatic techniques were introduced into problems of collective phenomena in a classical context—the cluster expansions—the modern techniques had their root in work on quantum electrodynamics after the Second World War. As we have seen, these techniques grew independently in the study of the electron gas and of nuclear matter, were extended to finite temperature by Matsubara and others,⁵³⁷ were first applied to neutral Fermi systems by Migdal and Galitskii,⁵³⁸ and were then applied to superconductivity by Gor'kov and to helium by Beliaev and by Hugenholtz and Pines.⁵³⁹

The war aided this development by providing experimental technologies that contributed to the development of quantum electrodynamics,⁵⁴⁰ by increasing the funding for solid-state physics (Chapter 9), and by making it fashionable for those talented in physics and mathematics to enter solid state and work on applied problems. By the 1950s, solid-state theory had clearly developed from an area in which practitioners worked on rather abstract problems of ideal solids (Chapter 2) to one in which physicists could deal with the physics of solids.

The connection of the many-body problem to field theory helped as well to fertilize high-energy physics. For example, the concept of broken symmetry and the accompanying Anderson–Higgs mechanism has played a major role in theories of elementary particles, such as the unified theory of electroweak interactions. Just as solid-state physics had been a proving ground for quantum mechanics in the late 1920s and early 1930s (Chapter 2), collective phenomena problems would eventually serve as a source of ideas as well as a testing ground for quantum field theory.

By the late 1950s, approaches to collective phenomena in different physical contexts—the electron gas, superconductivity, helium, and nuclear matter—had converged sufficiently to define a field of "many-body physics." An international community working on various aspects of the problem had formed and begun to meet regularly at specialized conferences and to train students. The first major symposium on the many-body problem was held in January 1957, at the Stevens Institute of Technology, where relationships between theoretical work in these various areas were examined and put into perspective. The Les Houches summer school of 1958, entitled "The Many-body Problem" and organized by Nozières, included courses by Schrieffer on the theory of superconductivity; Huang on the hard-sphere boson gas and the binary collision approach of Lee and Yang; Brueckner on the application of many-body theory to nuclear matter and other problems; Bohm on collective coordinates; Pines on electrons, plasmons, and phonons; Beliaev on the Bogoliubov canonical transformation method; and Hugenholtz on perturbation theory of many-fermion systems.⁵⁴¹ The second major meeting on the many-body problem, held at Utrecht in June 1960 and attended by several leading Soviet physicists,

added phase changes, a problem of continuing interest in the Netherlands, to the topics covered at the Stevens meeting.⁵⁴²

Until the 1960s, phase transitions remained somewhat apart from the streams that converged into many-body physics. However, as superconductivity and superfluidity became better understood, the attention of many-body physicists began to turn to applications of their proven methods to problems of critical phenomena. Important examples were the studies of the critical behavior of superfluid ⁴He by Patashinskii and Pokrovskii, and by Josephson.⁵⁴³ With the development of renormalization group techniques starting in the mid-1960s, this area too came under the umbrella, and the study of collective phenomena had come together as a single area of the physics of condensed matter.

Notes

S. Heims is the major author of the sections on phase transitions and critical phenomena, and H. Schubert is responsible for the sections on liquid helium and the prewar history of superconductivity. The discussion of the post-BCS period in superconductivity is based in large part on an unpublished manuscript of P. W. Anderson, "It's Not Over till the Fat Lady Sings," presented at the March 1987 meeting of the American Physical Society, New York City. We would like to thank Professor Anderson for making this manuscript available to us for use in this chapter.

1. See, for example, F. Bloch, *Die Elektronentheorie der Metalle, Handbuch der Radiologie*, 2nd ed. (Leipzig: Akademische Verlagsgesellschaft, 1933), 6: pt. 1, 226–278, 238–239, 278; Bloch, "Some Remarks on the Theory of Superconductivity," *Physics Today* 19, no. 5 (1966): 27–36; L. Brillouin, *Die Quantenstatistik und ihre Anwendung auf die Elektronentheorie der Metalle*, vol. 13 of *Struktur der Materie in Einzeldarstellungen* (Berlin: Springer, 1931), intro., 45, 413–415; H. G. Smith and J. O. Wilhelm, "Superconductivity," *Reviews of Modern Physics* 7 (1935): 237–271, p. 270.

2. We would like to acknowledge very helpful discussions with John Bardeen, Anthony Leggett, Christopher Pethick, and David Pines in developing this history, as well as all those, named explicitly in the notes, whom we interviewed. All interviews referred to in this chapter have been deposited at AIP unless otherwise indicated. For their critical reading of the entire chapter, and numerous corrections and additions, we are particularly grateful to Spencer Weart, David Pines, and Philip Anderson. These readers also made many valuable suggestions of areas in which the material deserves further expansion; we regret that project deadlines and space limited the extent to which we were able to add such material in appropriate detail. Scientific areas that have strongly influenced many-body theory and certainly warrant expanded treatment include quantum transport in solids and the collective theory of magnetism; it was unfortunately not possible to include the latter in Chapter 6 either. Valuable historical sources in these areas are Anderson's interviews with Hoddeson on 13 July 1987 and 10 May 1988, as well as his letter to Hoddeson of 11 February 1988 (all on file at the Center for History of Physics at the AIP), and his article "Some Memories of Developments in the Theory of Magnetism," *Journal of Applied Physics* 50, no. 11 (1979): 7281–7284. We also recognize that the present history does not, for lack of access to primary documents, adequately treat Soviet or Japanese contributions to the modern development of the theory of collective phenomena; we look forward to more complete material from Soviet and Japanese historians of solid-state physics.

3. The principal elementary excitations in the theory of collective phenomena are the following: the phonon, which is a quantum of lattice vibration above the ground state in a crystal, or a long-wavelength-density oscillation in liquid ⁴He; the quantized spin wave in a ferromagnet, or magnon (Chapters 2 and 6); the exciton, or bound electron–hole in an insulator or a semiconductor (Chapter 4); the polaron, an electron moving through a polar crystal lattice "dressed" by the comoving

Mechanics (New York: Benjamin, 1962); A. A. Abrikosov, I. E. Dzyaloshinskii, and L. P. Gor'kov, *Methods of Quantum Field Theory in Statistical Physics* (Moscow: Fizmatgiz, 1961; New York: Prentice-Hall, 1963). Further references may be found in Pines (n. 520).

524. Wilson, in Domb and Green (n. 518).

525. F. Bloch, interview with T. Kuhn, 14 May 1964; R. Peierls, interview with J. L. Heilbron, 17 June 1963, Archives for the History of Quantum Physics, American Philosophical Society, Philadelphia, copies at AIP and elsewhere.

526. Schweber (1989) (n. 242).

527. For a descriptive summary, see D. Pines, "Elementary Excitations in Quantum Liquids," *Physics Today* 34, no. 11 (1981): 106–131.

528. Bloch (n. 183).

529. Landau (n. 182).

530. Ginzburg and Landau (n. 302).

531. Gor'kov (n. 403).

532. London (n. 135).

533. O. Penrose, "On the Quantum Mechanics of Helium II," *Phil. Mag.* 42 (1951): 1373–1377. See also Penrose and Onsager (n. 455).

534. Pitaevskii (n. 457); Gross (n. 457).

535. Josephson (n. 409); Pippard (n. 384); Anderson ("It's Not Over") (n. 382).

536. C. N. Yang, "Concept of Off-Diagonal Long-Range Order and the Quantum Phases of Liquid He and of Superconductors," *Reviews of Modern Physics* 34 (1962): 694–704.

537. See nn. 273, 274, 277, 522, 523.

538. Galitskii (n. 462); Galitskii and Migdal (n. 462).

539. Gor'kov (n. 403); Beliaev (n. 456).

540. P. Galison, "Impact of World War II on Postwar Particle Physics" (contribution to the Los Alamos Symposium on Transfer of Technology from World War II to Postwar Science, May 1987, ed. R. Seidel [to be published]); Schweber (n. 242).

541. *The Many Body Problem*, Proceedings of Les Houches summer school, 1958 (London: Methuen, 1959).

542. Early texts on the many-body problem include D. ter Haar, *Introduction to the Physics of Many-body Systems* (New York: Wiley Interscience, 1958); Pines (n. 520); Abrikosov et al. (n. 523); Kadanoff and Baym (n. 523).

543. Pathashinskii and Pokrovskii (n. 518); Josephson (n. 518).